

Succinic acid, 4-chloro-2-nitrobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H24ClNO6/c1-4-5-16(12(2)3)26-18(22)9-8-17(21)25-11-13-6-7-14(19)10-1
InchiKey:	UMXFQQLHPLYAFP-UHFFFAOYSA-N
Formula:	C18H24ClNO6
SMILES:	CCCC(OC(=O)CCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-])C(C)C
Mol. weight [g/mol]:	385.84

Physical Properties

Property code	Value	Unit	Source
gf	-255.27	kJ/mol	Joback Method
hf	-727.92	kJ/mol	Joback Method
hfus	49.72	kJ/mol	Joback Method
hvap	97.77	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.439		Crippen Method
mvol	285.260	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2592.00		NIST Webbook
rinpol	2592.00		NIST Webbook
tb	988.85	K	Joback Method
tc	1220.58	K	Joback Method
tf	631.93	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.67	J/mol×K	988.85	Joback Method
cpg	901.63	J/mol×K	1027.47	Joback Method
cpg	911.24	J/mol×K	1066.09	Joback Method
cpg	919.51	J/mol×K	1104.71	Joback Method
cpg	926.48	J/mol×K	1143.34	Joback Method
cpg	932.17	J/mol×K	1181.96	Joback Method
cpg	936.61	J/mol×K	1220.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380939&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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